Composite particles in quantum chemistry: from two-electron bonds to cold atoms

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Ab initio quantum chemistry usually treats electrons as elementary particles, thus the theory of *composite particles* is absent from most textbooks. However, we do deal with composite particles implicitly, e.g., when considering nuclei as point-like, structureless objects. This is a trivial limiting case, as the internal interactions between hadrons gluing together the nuclei are so strong that no chemical process is comparable. Consequently, the only point where the composite nature of a nucleus enters is the counting of its total spin.

Forming composite particles from electrons is a much less trivial problem, since the binding forces between them may easily be affected by external interactions. Such composites form the basis of certain *models*, among which the BCS theory of Cooper pairs is perhaps the most successful. Another example is to consider a localized two-electron chemical bond as a composite particle, which is clearly a fragile object. In the latter case the term *composite quasi-particle* seems to be more adequate.

Distinguishing between true elementary particles and composite quasi-particles can be done most thoroughly by studying the commutation properties of their creation and annihilation operators. Quasi-particles always exhibit a complicated algebra, in contrast to elementary particles which commute or anticommute to unity in the case of bosons or fermions, respectively. A challenge here is to make predictions on the validity of the quasi-particle approximation based on the mathematical form of commutators. Another important issue is to develop correction schemes which describe the effect of the internal structure of quasi-particles on their interactions.

Going to larger composites, some applications permit one to treat a whole atom as a single particle. Approximating an atom as an elementary particle may also be permitted sometimes. The success of the Bose-Hubbard model of cold, dilute atomic gases represents such an example. Solution of the Bose-Hubbard model is another challenging field where quantum chemical techniques may find applications.

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